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Educations

Argonne National Laboratory

04/2018 - present

Postdoctoral

Kansas State University

08/2013 – 02/2018

PhD in Chemical Engineering

Beijing University of Chemical Technology

09/2009 – 06/2013

B.S. in Chemical Engineering and Technology Dissertation

Research Experiences

Argonne National Laboratory

04/2018 – present

Project:

Computational modeling of aldol condensation and ketonization on metal oxide and metal carbide surfaces

Kansas State University

08/2013 – 02/2018

Project:

First-principles modeling of water-gas shift reaction on transition metals couple with microkinetic simulations

Peer-Reviewed Journal Publications

1. **Mingxia Zhou**, Lei Cheng, Jae-Soon Choi, Bin Liu, Rajeev S. Assary, and Larry A. Curtiss, Ni-Doping Effects on Oxygen Removal from an Orthorhombic Mo₂C(001) surface: A Density Functional Theory Study. **J. Phys. Chem. C**, 2018, 122, 3, 1595-1603.
2. Wenshuai Zhu, Zili Wu, Guo Shiou Foo, Xiang Gao, **Mingxia Zhou**, Bin Liu, Gabriel M. Veith, Peiwen Wu, Katie L. Browning, Ho Nyung Lee, Huaming Li, Sheng Dai, and Huiyuan Zhu, Taming interfacial electronic properties of Pt nanoparticles on vacancy-abundant boron nitride nanosheets for enhanced catalysis. **Nature Communications**. 2017, DOI: 10.1038/ncomms15291.
3. **Mingxia Zhou**, and Bin Liu, A first-principles investigation of adsorbate-adsorbate interactions on Ni(111), Ni(211), and Ni(100) surfaces. **Ind. Eng. Chem. Res.** 2017, DOI: 10.1021/acs.iecr.7b00447.
4. **Mingxia Zhou**, Thong Nguyen-Minh Le, Lam K. Huynh, and Bin Liu, Effects of Structure and Size of Ni nanocatalysts on Hydrogen Selectivity via Water-gas-shift Reaction – A First-principles-based Kinetic Study. **Catalysis Today**. 2017, 280, 210-219.
5. Nannan Shan, **Mingxia Zhou**, Mary K. Hanchett, Josephine Chen & Bin Liu, Practical principles of density functional theory for catalytic reaction simulations on metal surfaces – from theory to applications. **Molecular Simulation**. 2017, DOI:10.1080/08927022.2017.1303687.
6. **Mingxia Zhou** and Bin Liu, DFT Investigation on the Competition of the Water-Gas Shift Reaction Versus Methanation on Clean and Potassium-Modified Nickel(111) Surface. **ChemCatChem**. 2015, 7, 3928-3935.
7. Bin Liu, **Mingxia Zhou**, Maria K. Y. Chan, and Jeffrey P. Greeley, Understanding Polyol Decomposition on Bimetallic Pt-Mo Catalysts – A DFT Study of Glycerol. **ACS Catal.** 2015, 5, 4942-4950.